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Final Project Report: Design of Heterogeneous Heat Conducting and Elastic Structures with Imperfect Interface, AFOSR Grant F49620-96-1-0055

Robert P. Lipton.

Abstract

The results obtained in this project predict novel physical phenomena for multiphase systems that are imperfectly bonded or have bonds with better transport properties than any of the constituent materials. These results are unlike phenomena seen in more traditional treatments where the interface between constituents is treated as a "perfect bond". The difference is that sample and particle size effects are predicted, where as "perfect bond" models are incapable of capturing this physically observed phenomena. In addition to capturing the "size effect," the new mathematical methods developed in this project provide a systematic way for predicting new "size effects". These results have direct application to rigorous design rules for particle and fiber reinforced composite structures. The structures and reinforcements that can be treated using this new mathematical approach range from the very small scale (nanometers) to the very large scale (kilometers).

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1 Research overview.

The characterization of multiphase solid and fluid systems is central to the design of materials for use in the applications; these include the design of semiconductor packaging materials, the characterization of ceramic materials for use in thermal barrier coatings, the design of large scale concrete structures, and new materials for use in antenna design.

This project studies the effect of the interface on the transport properties of a composite material. In the contexts of heat conduction or dc electric transport the interface between two phases may exhibit a contact resistance, or carry a surface flux. In the context of elasticity we consider the case where there is a jump in the tangential displacement across the interface. This type of interface condition may arise due to damage of the composite structure during service. In porous ceramics heat and mass transport are coupled by a chemical reaction on the pore surface. This project addresses each of the aforementioned types of interface transport.

The methods used as well as the scope of this project are inherently different from more traditional approaches where the interface between constituents is treated as a "perfect bond." In the standard treatment of perfectly bonded materials a separation of macroscopic and microscopic scales is assumed. The resulting effective macroscopic transport properties obtained by homogenization contain no information on the actual size of the small scale structure. In fact, for periodic microstructures the macroscopic properties are easily seen to be invariant under a re-scaling of the microstructure. On the other hand, most composite materials contain heterogeneities at both microscopic and macroscopic length scales, and the actual size of the heterogeneity effects the transport properties of the composite material. The approach taken in this project differs with that of previous investigations in two distinct ways: the first is that heterogeneities are not assumed small with respect to the dimensions of the domain occupied by the composite material, and the second is that the effect of the interface is considered.

In order to elucidate the ramifications of interfacial transport a new set of mathematical tools is required. One of the basic questions associated with the effect of the interface is the question of existence of a critical length scale for which the effects of the interface overwhelm the transport properties of the bulk phase. During the course of this project I have introduced new mathematical tools to answer this question. One such set of tools are new Poincare-like inequalities that allow one to estimate the energy dissipated inside a region in terms of the energy dissipated on the interfacial surface

surrounding it. I have shown that the best constant for such inequalities contains the relevant geometric information giving the length scale at which the effects of the interface dominate the transport properties of the bulk phase. For certain imperfect interface conditions, these constants are given by the first nonzero eigenvalue coming from the classical Stekloff eigenvalue problem. While for other interface conditions the constants are associated with new eigenvalue problems involving both the Laplace-Beltrami operator on the interface and the Calderon operator associated with the bulk phase. Application of these methods provides a systematic way for finding new sample and particle size effects for the transport properties of composite materials. The traditional "perfect bond" models are incapable modeling or predicting size effect phenomena.

The results obtained in this project have delivered rigorous design rules for particle and fiber reinforced composite structures. In the context of imperfectly bonded elastic materials the methods presented here provide for the robust design of structures that are expected to sustain damage during service. Here no separation of scales is assumed and the structures and reinforcements that can be treated using the new mathematical approach, range from the very small scale (nanometers) to the very large scale (kilometers).

2 Grant sponsored projects completed.

- **Energy dissipation inequalities for functionals with surface energy and new size effects for particle and fiber reinforced thermal conductors.**

A functional with both bulk and interfacial surface energy is considered. It corresponds to the energy dissipated inside a two-phase heat conductor in the presence of a thermal contact resistance at the two-phase interface. The second Stekloff eigenvalue associated with the reinforcement phase is shown to be a basic tool for the study of non-local perturbations of functionals with bulk and surface energies associated with imperfectly bonded composite conductors. The effect of embedding a highly conducting particle into a matrix of lesser conductivity is investigated. The geometric criterion that determines when the surface energy becomes larger than the bulk energy inside the particle is found. This criterion is general and applies to any particle with Lipschitz continuous boundary. It is given in terms of the of the second Stekloff eigenvalue ρ_2 of the particle. This result provides a

new link between particle geometry and the thermal energy dissipated inside a particle reinforced heat conductor. In this context, the second Stekloff eigenvalue is the ratio measuring the relative importance between the particle's ability to dissipate heat and the total heat flux passing through the boundary of the particle. For a spherical particle of unit conductivity, this quantity is precisely the reciprocal of the radius of the sphere. For particles of general shape this quantity can be estimated in terms of the dimensions of the particle. The criterion is given in terms of a number R_{cr} that is the ratio between the thermal barrier resistance and the contrast between the resistivities of the particle and matrix phases. It is shown that the particle will not reduce the overall energy dissipation if :

$$c_p \rho_2^{-1} \leq R_{cr} \quad (1)$$

Here c_p is the particle conductivity. It is stressed that this criterion holds independently of the location and shape of the remaining particles in the suspension. This result is used to provide new mathematical guidelines for the design of particle reinforced conductors with minimum energy dissipation.

These tools are used to predict existence of energy minimizing configurations for particle reinforced conductors. It is shown that fine scale oscillations are rendered superfluous due to the thermal barrier associated with the interface.

- **Design of particle reinforced heat conducting composites with interfacial thermal barriers**

The new criterion derived in the previous work is used to provide new design rules for particle and fiber reinforced structures. This criterion is given in terms of the parameter: $R_{cr} = \beta^{-1}(c_m^{-1} - c_p^{-1})^{-1}$. Here matrix and particle conductivities are given by c_m and c_p respectively. The contact resistance is characterized by the scalar β having the dimensions of conductivity per unit length. The parameter R_{cr} has dimensions of length. New rigorous design rules are given for particle reinforced suspensions with least energy dissipation. As an example we consider suspensions of cylindrical fibers of length ℓ and radius R . For long slender fibers ($\ell/2 \geq R$), filled with isotropic conductor, we find that any particular fiber will not reduce the total energy dissipated in the composite when: $R_{cr} \geq \frac{((\ell/2)^2 + R^2)^2}{R^3}$. Similar remarks can be made

for penny shaped fibers where $\ell/2 \leq R$ and for ellipsoidal inclusions. For spherical particles in an isotropic matrix, we find that the energy dissipation is not reduced when the particle radius drops below R_{cr} . The scale of the size effect is set by the value of R_{cr} . Depending upon the values of the interfacial thermal resistance and the constituent resistivities this value can range from nanometers to geologic length scales.

- **Influence of interfacial surface conduction on the dc electrical conductivity of particle reinforced composites** We consider a particle reinforced composite. The case when electrical conduction occurs along phase interfaces, as well as inside the particle and matrix phases, is addressed. For particles with Lipschitz boundary, a new quantity called the *surface to volume dissipation* of a particle is introduced. This quantity is a measure of the particle's ability to dissipate energy on its surface relative to the energy dissipated in its interior. It is described mathematically as the minimum value of a suitably defined Rayleigh quotient, and is related to a novel eigenvalue problem posed on the particle surface. The eigenvalue problem is given in terms of the Laplace-Beltrami operator on the particle surface and the Calderón operator associated with the region occupied by the particle. We consider the overall conductivity of a particle reinforced conductor when the particle conductivities are less than that of the matrix. It is shown that the overall conductivity will be increased by the presence of a specific particle when the particle's "surface to volume dissipation" lies above a critical value. We calculate the surface to volume dissipation for a sphere and for starlike particles we provide a lower bound in terms of particle dimensions. These bounds predict the existence of critical particle dimensions below which the particle will always increase the overall conductivity of the composite. These results show that under the right conditions, the presence of interfacial conducting paths will increase the overall conductivity beyond that of the matrix phase even below the interfacial percolation threshold.

One practical application of the physico-mathematical model treated here is the modeling of ionic diffusion in concrete. This phenomenon is important as ions react with steel reinforcements in the concrete, corroding them and compromising the overall structural properties. In light of the Nerst-Einstein relation there is a direct relation between the DC electrical conductivity of concrete and the ionic diffusivity.

- Design of imperfectly bonded fiber reinforced shafts for maximum torsional rigidity.

A tight upper bound on the torsional rigidity for a large class of fiber shapes and fiber-shaft configurations is established. The interfacial bonding stiffness per unit length is denoted by α and the shear moduli of the matrix and fibers is given by G_m and G_f respectively. The fibers provide reinforcement, hence $G_f > G_m$. We consider the set of shafts with prescribed cross-sectional area, reinforced with at most N fibers with simply connected cross sections. The fiber cross sections are denoted by $\Sigma_1, \Sigma_2, \dots, \Sigma_N$, and the area occupied by the i^{th} fiber cross section is written $|\Sigma_i|$. We have the following tight upper bound:

If the surface traction to bulk stress quotient of each fiber cross-section lies above $\frac{\alpha^{-1}}{G_m^{-1}-G_f^{-1}}$, then the torsional rigidity is less than or equal to the torsional rigidity of a concentric circular fiber-shaft configuration.

where the radius "a" of the circular fiber is given by:

$$\pi a^2 = \sqrt{|\Sigma_1|^2 + |\Sigma_2|^2 + \cdots + |\Sigma_N|^2}. \quad (2)$$

It is evident from (2) and the inequality,

$$\sqrt{|\Sigma_1|^2 + |\Sigma_2|^2 + \cdots + |\Sigma_N|^2} \leq |\Sigma_1| + |\Sigma_2| + \cdots + |\Sigma_N|, \quad (3)$$

that the cross-sectional area of the circular fiber is less than or equal to the joint cross-sectional area of the fiber configuration.

• Isoperimetric Inequalities for Torsional Rigidity

We consider prismatic shafts with shear stiffness G_m reinforced with fibers of greater shear stiffness G_f . The fibers are assumed to be imperfectly bonded to the shaft. The degree of imperfect bonding is characterized by an interfacial shear stiffness α . We consider all shaft cross sections of the same cross-sectional area and consider all reinforcements of N fibers of given joint cross-sectional area. We suppose that each fiber cross section may be multiply connected.

For simple fiber-shaft configurations the torsional rigidity can be calculated explicitly. Indeed, calculation shows that the torsional rigidity associated with circular shaft composed of a centered circular cross section of compliant material with radius a , surrounded by an annular fiber of stiff material with outer radius R is given by:

$$\frac{\pi G_f}{2}(R^4 - a^4) + \frac{\pi G_m}{2}a^4$$

The main result of this project is the following isoperimetric inequality:

Isoperimetric inequality

Of all fiber reinforced shafts with prescribed cross-sectional area, reinforced with at most N multiply connected fibers with given joint cross-sectional area, the shaft with circular cross section composed of a centered circular cross section of compliant material reinforced with an outer annular fiber of stiff material has the maximum torsional rigidity.

Let the πa^2 be the joint area of the more compliant material and πR^2 be the area of the shaft cross-section. Then the theorem asserts that the torsional rigidity is always less than or equal the value:

$$\frac{\pi G_f}{2}(R^4 - a^4) + \frac{\pi G_m}{2}a^4$$

This result complements the previously reported work for fiber reinforced shafts where each fiber cross section is constrained to be to be simply connected.

Most often the geometry of a structural composite is not fully specified. Instead only partial statistical information is available. For example, the geometry of a particle reinforced composite may only be specified by the particle size distribution and particle volume fraction. Other parameters describing the degree to which the particles are clumped together may also be known. In this context, the goal is to understand how the transport properties depend upon the limited statistical information in the presence of imperfect or nonstandard interface conditions. The approach that I have taken is variational and is not tied to a particular composite geometry, approximate formula, or dilute approximation. The tools that I have developed for these problems are new variational principles from which bounds on the effective properties are obtained through simple choices of trial fields. The attractive feature is that any observation deduced from the bounds is not tied to a particular geometry or approximate formula and will apply to any statistically defined composite system. Bounds derived in this way provide new rigorous mathematical guidelines for the design of particle reinforced composites when only statistical data on the particle configuration is available. During the course of this project I have been able to extend these methods to situations when there is coupled physics at the two-phase interface.

- **Variational methods bounds and size effects for composites with highly conducting interface.**

New variational principles are introduced describing the effective conductivity tensor for two phase electric conductors. The interface between the conductors is assumed to be highly conducting. Extra geometric information is encoded into the variational principles through the solution operators of simpler transport problems. These operators can be expressed as gradients of simple layer potentials with densities

supported on phase interfaces or in terms of simple Dirichlet problems inside each phase region. The approach taken here is motivated by the idea that variational principles containing extra geometric information provide tighter bounds than those obtainable from the more standard Dirichlet or Thompson-like variational principles for any given class of trial fields. New upper bounds on the effective conductivity for particulate composites are found that depend upon component volume fractions, a surface energy tensor, and a scale free matrix of parameters. This matrix corresponds to the effective conductivity tensor associated with the same geometry but with perfectly conducting inclusions. New lower bounds are given in terms of two point correlation functions, component volume fractions, and interfacial geometric parameters. Both upper and lower bounds are found to be optimal for certain choices of interfacial geometric parameters.

These bounds provide the tools necessary for the identification of new particle size effects. As an example, we consider isotropic suspensions of particles with conductivity less than that of the matrix. The matrix, particle, and effective conductivity are denoted by c_m , c_p , and c_e respectively. The volume fraction of particles is denoted by θ_p and no assumptions on the distribution of particle size and shape in the suspension are made. It is shown that the effective conductivity is less than that of the matrix provided that the interfacial surface area is less than the quantity $3\theta_p P_{cr}^{-1}$, where $P_{cr} = 2\alpha(c_m - c_p)^{-1}$. Polydisperse suspensions made from isotropic conducting spheres of different radii embedded in a matrix of isotropic conductivity are considered. The distribution of sphere radii within the suspension is given. The probability measure associated with the distribution of sphere radii is denoted by $P(a)$ and the mean of the reciprocal radii is $\langle a^{-1} \rangle = \int_0^\infty a^{-1} dP(a)$. The mean radius is $\langle a \rangle = \int_0^\infty a dP(a)$. For isotropic suspensions we obtain the inequalities:

$$\text{if } \langle a^{-1} \rangle^{-1} \geq P_{cr} \text{ then, } c_e \leq c_m \text{ and if } \langle a \rangle \leq P_{cr} \text{ then, } c_e \geq c_m. \quad (4)$$

- **Variational Methods, Bounds, and Size Effects for Two-phase Composites with Coupled Heat and Mass Transport Processes at the Two-phase Interface**

New variational principles are developed for the overall heat transport of anisotropic two-phase particle reinforced composites in the pres-

ence of coupled mass and heat transport processes at the two-phase interface. We focus on physical situations where an imposed temperature gradient causes impurities or lattice defects to concentrate on the two-phase interface and diffuse along it. This is accompanied by the release and absorption of heat as the impurities respectively enter or leave the interface. The treatment given here predicts for the first time, new size effects, critical radii, and energy dissipation inequalities for heat conduction in the presence of coupled heat and mass transport processes at the two phase interface. These results translate into rigorous rules of thumb on the pore size distribution for the optimal design of porous ceramics.

In this project new Dirichlet and Thompson-like variational principles describing the effective thermal conductivity σ^e are derived. From these we build two more variational principles that implicitly contain extra information on the composite geometry. The approach here is also motivated by the idea that variational principles containing extra geometric information provide tighter bounds than those obtainable from the Dirichlet or Thompson-like variational principles for any given class of trial fields. The variational principles introduced here incorporate geometric information through the solution operators of simpler comparison problems. These operators admit an explicit representation either in terms of gradients of simple layer potentials supported on the pore-matrix interface, projection operators on the space $L^2(\Omega)^3$, or are associated with simple Dirichlet or Neumann problems in each phase.

We substitute simple trial fields into the variational principles to obtain new bounds on the overall thermal conductivity of the composite. The bounds are used to investigate the effect of the inclusion geometry on the overall thermal conductivity. For randomly distributed inclusions new rigorous rules of thumb are given for the design of composites with desirable overall heat conduction. For spherical inclusions, these rules of thumb are given in terms of the inclusion size distribution and nearest neighbor distribution function for the inclusions. New dimensionless parameters are found that mediate the overall thermal transport properties. For inclusions of general shape, these parameters are given in terms of material transport properties for the bulk and interfacial phases together with the average *surface to volume dissipation* of the inclusions and the nearest neighbor distribution function

for the inclusions.

The methods used in this project are variational in nature and allow one to treat the problem directly without approximating the field interactions between pores. The results given in this work corroborate the anomalous behavior of the effective thermal conductivity with temperature as reported in [Gambaryan, T., Litovsky, E., and Shapiro, M. 1993 Influence of segregation-diffusion processes on the effective thermal conductivity of porous ceramics. *Int. J. Heat Mass Transfer* 36, 4123-4131].

3 Work at Air Force laboratories.

I have been interacting with Rollie Dutton at Wright Patterson AFB. Dr. Dutton is interested in the thermal and elastic properties of plasma sprayed ceramic thermal barrier coatings as a function of the local composite morphology. Such coatings are used in high performance gas turbine engines. My role in the project is to provide a model for the overall thermal conductivity based on the physics that is occurring in the thermal barrier coating. Given that the geometry of the grains and the imperfect interfaces can only be partially specified statistically, the goal of my project is to provide useful bounds on the overall conductivity in terms of the partial statistics of the composite. Once the bounds have been deduced - they will be used to predict the evolution of overall properties as a portion of the splat interfaces change from imperfectly bonded to perfectly bonded. The idea is to see if we can explain the experimental results or to come up with a plausible scenario under which we could expect new phenomena. (The experiments are currently in progress.) A second use for the bounds will be to rule in the possibility of experimental measurement error.

The next step in the project is to determine the Young's modulus of the barrier coating as a function of the imperfect bonding at splat interfaces. Knowledge of the Young's modulus predicts the onset of stress concentrations and the resulting de-bonding of the thermal barrier from the substrate. This knowledge would be useful input for estimating the lifetime of the thermal barrier coating.

4 Publications from grant sponsored activity given a Featured Review in Mathematical Reviews

Lipton R. "Variational methods, bounds, and size effects for composites with highly conducting interface," *Journal of the Mechanics and Physics of Solids*, vol. 45, no. 3, 1997, pp. 361-384. 1998 Mathematical Reviews reference number: 98c:73007.

5 Publications resulting from grant sponsored activity.

- Lipton R. "The second Stekloff eigenvalue and energy dissipation inequalities for functionals with surface energy," *SIAM Journal on Analysis*, 29 (1998), pp. 673-680.
- Lipton R. "Influence of interfacial surface conduction on the DC electrical conductivity of particle reinforced composites," *Proceedings of the Royal Society of London Ser. A*, 454 (1998), pp. 1371-1382.
- Lipton R. "Optimal fiber configurations for maximum torsional rigidity," *Archive for Rational Mechanics and Analysis*, 144 (1998), pp. 79-106.
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- Lipton R. "Variational methods, bounds, and size effects for two-phase composites with coupled heat and mass transport process at the two-phase interface. To appear in Journal of the Mechanics and Physics of Solids 1999.